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Energy-level calculation through modified Hill determinant approach : for general oscillator

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Abstract A method for calculation of energy levels using the modified Hill determinant approach has been developed An example of this approach is given for the general oscillator $V(X) = \lambda_1 X^2 + \lambda_2 X^4 + \lambda_3 X^6$ Very accurate convergent energy levels are presented

Keywords Energy-level calculation, Hill determinant approach, general oscillator

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1. Introduction

In quantum mechanics, as in classical mechanics, there are relatively few systems of physical interest for which equations of motion yield exact solutions. In practice, since the exactly solvable problems are rare, one must frequently resort to approximations. This has culminated in the development of many useful approximation techniques, some perturbative and some nonperturbative. Among the nonperturbative approximations, one has for example, the Hill determinant [1], the two-step procedure [2], the operator method [3], various 1/N expansions for spherically symmetric potentials [4], the rational function approach [5], the multiple-step recursion approach [6], supersymmetric quantum mechanics-based methods [7], and variational approach [8]. Almost all these methods use the anharmonic oscillator Hamiltonian

$$H = P^2 + X^2 + \lambda X^4 \tag{1}$$

as an example, not only because of its important applications in quantum field theory and molecular physics [9] but also because of the work of Bender and Wu [10] who have shown

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that the perturbation expansion for the energy level $E_n(\lambda)$ is not convergent. The eigenvalues of the anharmonic oscillator of the type λX^{2n} have been calculated by Biswas *et al* [1] with great success using the Hill determinant approach. Later on, it was pointed out [11-16] that the method [1] has a limited domain of applicability in the plane of couplings for the sextic oscillator

$$V(X) = \lambda_1 X^2 + \lambda_2 X^4 + \lambda_3 X^6, \quad \lambda_3 > 0 .$$

It has been shown [13-15] that the method of Singh, *et al* [17] fails to produce correct eigenvalues for the potential $V(X) = -2X^2 - 2X^4 + X^6$. Chaudhuri and Mondal [16] have calculated the first four energy levels of this oscillator by introducing a variational parameter in the Hill determinant approach following the operator method of Feranchuk and Komarov [3]. Killingbeck [15] has calculated energy levels of this oscillator by introducing a variational parameter in the exponential convergence factor of the wave function. Recently, Agarwal and Varma [18] have shown that it is necessary to introduce a modification on the method of Hill determinants by Chaudhuri and Mondal [16] which incorporates the operator method of Feranchuk and Komarov [3]. Further we find that even the low-lying energy levels calculated by Chaudhuri and Mondal [16] are not exactly the same as those reported by Killingbeck [15]. Hence, we feel that there is a need for generalizing the Hill determinant approach for a general oscillator Hamiltonian.

In this communication, we generalize the Hill determinant approach.

2. Hill determinant method

The Hamiltonian under consideration is defined by the relation

$$H = \mu T + V(q), \tag{2}$$

where

$$V(q) = CB(q) + \lambda_1 H_1(q) + \lambda_2 H_2(q) + \lambda_3 H_3(q) + \ldots$$

$$= CB(q) + \sum_{l=1}^{N} \lambda_l H_l(q) . \tag{3}$$

In the above, T is the kinetic energy, $CB(q)$ is the unperturbed potential, $\sum_{l=1}^{N} \lambda_l H_l(q)$ represents the perturbation term and μ is a dimensionless constant. The unperturbed Hamiltonian

$$H_C = \mu \left[T + \frac{CB(q)}{\mu} \right] \tag{4}$$

satisfies the eigenvalue relation

$$H_C | n >_C = \mu E_n(C) | n >_C , \tag{5}$$

where $E_n(C)$ is the n-th unperturbed energy and $| n >_C$ is the corresponding n-th eigenfunction. Now we shift the parameter C to a new parameter C_1 where

$$C_1 = \frac{C}{\mu} + \sum_{l=1}^{N} \lambda_l \alpha_l \frac{< g | H_l(q) | g >_{C_1}}{< g | \mu B(q) | g >_{C_1}} . \tag{6}$$

Hence, the new unperturbed Hamiltonian E_{C_1} satisfies the eigenvalue relation.

$$H_{C_1} | n >_{C_1} = \mu \left[T + C_1 B(q) \right] n >_{C_1} \tag{7}$$

The function $| n >_{C_1}$ can be obtained directly from the unperturbed function $| n >_C$ by replacing C by C_1. In the above, $| g >_{C_1}$ stands for the groundstate wave function of H_{C_1}. It is seen that in eq. (6) C_1 is also a function of C. Further, the contribution of C_1 is determined in terms of diagonal term of $H_l(q)$ without considering the non-diagonal contribution of $H_l(q)$. Hence, the contribution of non-diagonal part of $H_l(q)$ can be included through the parameter α_l. Therefore, we propose to determine α_l using the non-diagonal matrix elements of $H_l(q)$ through the parameter C as [19]

$$\sum_{m \neq g} \left[< g | H_1(q) | m > - \alpha_l \frac{< g | H_l(q) | g >}{< g | B(q) | g >} < g | B(q) | m > \right]_C = 0, \tag{8}$$

where suffix 'C' stands for unperturbed state in eq.(4). Further in eq.(8) the value of m to be considered for which the matrix elements $< g | H_l(q) | m >$ and $< g | B(q) | m >$ yield nonzero value. Hence, the original Hamiltonian in eq. (2) is rewritten as

$$H = H_{C_1} + H_{2D} + H_{2N}, \tag{9}$$

where H_{2D} and H_{2N} are the diagonal and the nondiagonal parts of

$$H_2 = \sum \lambda_1 \quad H_1(q) - \alpha_1 \frac{< g | H_l(q) | g >_{C_1}}{< g | B(q) | g >_C} \cdot B(q) \tag{10}$$

Now, we use orthonormal basis vector $| m >_{C_1}$ to express the wave function Ψ as

$$\Psi = \sum_{m=0} A_m | m >_{C_1} \tag{11}$$

and solve the eigenvalue equation

$$H\Psi = E\Psi. \tag{12}$$

3. Application

In order to make the procedure accessible to the reader, we apply it to the general oscillator characterized by the Hamiltonian

$$H = \mu p^2 + \lambda_1 X^2 + \lambda_2 X^4 + \lambda_3 X^6 \tag{13}$$

with ($\lambda_3 > 0$). The expression for H_W for the above Hamiltonian is

$$H_W = \mu \left(p^2 + W^2 X^2 \right), \tag{14}$$

where

$$W^2 = \frac{\lambda_1}{\mu} + \alpha_1 \frac{<0|\lambda_2 X^4|0>_W}{<0|\mu X^2|0>_W} + \alpha_2 \frac{<0|\lambda_3 X^6|0>_W}{<0|\mu X^2|0>_W}. \tag{15}$$

The value of α_1 is determined by the condition

$$\left[<0|X^4|2> - \alpha_1 \frac{<0|X^4|0>}{<0|X^2|0>} <0|X^2|2>\right] = 0 \tag{16}$$

on substituting $l = 1$ in eq. (8) and is found to be 2. Similarly by putting $l = 2$ in eq. (8), the value of α_2 is found to be 3. Hence, the parameter W satisfies the following quartic equation

$$4W^2\mu - 4\lambda_1 W^2 - 12\lambda_2 W - 45\lambda_3 = 0. \tag{17}$$

The expression for H_2 is

$$H_2 = \lambda_2\left[X^4 - \frac{3}{W}X^2\right] + \lambda_3\left[X^6 - \frac{45}{4W^2}X^2\right]. \tag{18}$$

Using eqs. (11, 12), one obtains the following recurrence relation that is satisfied by A_m.

$$P_m A_{m-6} + Q_m A_{m-4} + R_m A_{m-2} + S_m A_m + T_m A_{m+2} + U_m A_{m+4} + V_m A_{m+6} = 0, \tag{19}$$

where

$$P_m = \frac{\lambda_3}{8W^3}\left[m(m-1)(m-2)(m-3)(m-4)(m-5)\right]^{1/2}, \tag{19a}$$

$$Q_m = \left[\frac{3\lambda_3(2m-3)}{8W^3} + \frac{\lambda_2}{4W^2}\right]\left[m(m-1)(m-2)(m-3)\right]^{1/2}, \tag{19b}$$

$$R_m = \left[\frac{15\lambda_3(m+1)}{8W^3} + \frac{\lambda_2}{W^2}\right](m-2)\left[m(m-1)\right]^{1/2}, \tag{19c}$$

$$S_m = mW\mu + \frac{\lambda_1 m}{W} + \frac{6\lambda_2}{4W^2}(m^2+m) + \frac{\lambda_3}{8W^3}(20m^3+30m^2+40m)$$

$$+ \frac{W\mu}{2} + \frac{\lambda_1}{2W} + \frac{3\lambda_1}{4W^2} + \frac{15\lambda_3}{8W^3} - E, \tag{19d}$$

$$T_m = R_{m+2}, \tag{19e}$$

$$U_m = Q_{m+4}, \tag{19f}$$

$$V_m = P_{m+6}. \tag{19g}$$

The eigenvalue condition of the Hill determinant in the limit of large N is $\det D_N = 0$. With

$$D_N = \begin{pmatrix} S_n & T_n & U_n & V_n & 0.... \\ R_{n+2} & S_{n+2} & T_{n+2} & U_{n+2} & V_{n+2}.. \\ Q_{n+4} & R_{n+4} & S_{n+4} & T_{n+4} & U_{n+4}.. \\ P_{n+6} & Q_{n+6} & R_{n+6} & S_{n+6} & T_{n+6}.. \\ . & . & . & . & . \\ . & . & . & . & . \end{pmatrix} = 0, \tag{20}$$

where $n = 0$ for even parity eigenvalues and $n = 1$ for those of odd parity. The zeros of D_N as a function of the parameter E give the energy eigenvalues of the problem.

4. Comparison with some exact results

For any arbitrary values of λ_1, λ_2 and λ_3, it is impossible to find exact solution of the Hamiltonian in Eq. (13). However, for some specific values of λ_1, λ_3 with $\lambda_2 = 0$, one can solve it exactly. We

Table 1. Comparison with exact result

First two even levels	λ_3	λ_1	λ_2	Present				Previous [14]	
0	1	3	0	1 935	482	104	3	1 935	483
2				11 680	970	880	6		
0		2		1 697	2087	963	6	1 697	208
2				10 836	459	224	8		
0		1		1 435	624	618	9	1.435	625
2				9 966	622	001	9		
0		0		1 144	802	454	3	1.144	802
2				9 073	084	593	2		
0		-1		0 816	648	633	7	0 816	649
2				8 159	265	116	3		
0		-2		0 440	067	8831	3	0 440	068
2				7 231	201	533	8		
0		-3		0.000	000	000	0	0.000	000
2				6 298	495	944	2		
0		-1		-0 523	268	620	5	-0 523	269
2				5 374	970	019	7		
0		-5		-1 153	538	008	9	-1 153	538
2				4.478	041	420	3		
0		-6		-1.915	464	416	9	-1.915	464
2				3.625	337	212	7		
0		-7		-2.828	427	144	9	-2.828	427
2				2 828	427	040	6		
0		-8		-3 900	635	135	3	-3.900	635
2				2 086	528	041	3		
0		-11		-8.000	000	000	0		-8
2				0 000	000	000	0		

have compared the first two even states with the exact results of Tater and Turbiner [14] and find that in all the cases, present computed value yields good agreement (see Table 1).

5. Comparison between self-consistent and variational parameter calculation

In the previous examples, we find that the present self-consistent parameter C_1 when used in eq. (11) has yielded results that are in good agreement with the previous one. Let us consider another exactly solvable non-linear oscillator of the form [20-22]

$$H = P^2 + X^2 + X^2 < X^2 > . \tag{21}$$

Using present self-consistent method, we find that the parameter W satisfies the cubic equation

$$W^3 - W - 0.5 = 0 \tag{22}$$

and the ground state energy is

$$E_0 = W = 1.191\,487, \tag{23}$$

which remains the same as the exact one [20]. However, when variational principle is used, the parameter W satisfies the cubic equation

$$W^3 - W - 1 = 0 \tag{24}$$

and the ground state energy is found to be E_0 (variational) = 1.176 560. Hence, we find that the variational based calculation has failed in reproducing the correct ground state energy of the non-linear oscillator eq. (21).

6. Discussion

Apart from the comparison with the exactly solvable results in Table 1, we also present the first five (even and odd) convergent energy levels of the anharmonic oscillator $V(X) = \frac{X^2}{2} + X^4 (\mu = \frac{1}{2}, \lambda_1 = \frac{1}{2}, \lambda_2 = 1, \lambda_3 = 0)$ in Table 2 and compare the same with the 20-th order perturbation calculation by Caswell [23]. In this case, we have calculated the results

Table 2. The first five (even and odd) energy levels of the oscillator

$V(X) = \frac{X^2}{2} + X^4 (\mu = \frac{1}{2}, \lambda_1 = \frac{1}{2}, \lambda_2 = 1, \lambda_3 = 0)$

Levels	Present (even)					Previous [23]			
0	0.803	770	651	234	27	0 803	770	651	3
2	5 179	291	687	639	4	5 179	291	681	3
4	10 963	583	094	127		10 963	583	096	
6	17 634	049	116	138		17 634	049	115	
8	24 994	936	409	502		24 994	936	412	
Levels	Present (odd)					Previous [23]			
1	2 737	892	268	008	4	2 737	892	268	
3	7 942	403	984	391	0	7 942	404	...	
5	14 203	139	104	529		14.203	139	102	
7	21 236	435	486	758		21 236	435	489	
9	28.897	251	119	223		28.897	251	12	

for $N = 40$ and find that the results do not change even if N is increased upto $N = 400$. Present 12 decimal results are taken from the determinant size (80×80).

In the above case, the cubic equation has exact solution *i.e.* $W = 2$. However, for anharmonic oscillator $V(X) = X^2 + X^4 (\mu = \lambda_1 = \lambda_2 = 1, \lambda_3 = 0)$, we find cubic equation $W^3 - W - 3 = 0$ has a single positive root. Using $W = 1.671\ 699\ 8816$, we are able to reproduce values tabulated previously [24]. Similarly, for the quartic oscillator $V(X) = X^4$ using the value of $W = 1.4422495703074$, we are able to reproduce previous values [24]. In Table 3, we quote first five even parity and odd parity levels. Present results are from the size $N = 80$.

Table 3. First five even and odd energy levels of the $V(X) = X^2 + X^4$ and $V(X) = X^4$ (See Banerjee *et al* [24] for comparison)

Levels	Present $V(X) = X^2 + X^4$ W = 1 671 699 8816				Present $V(X) = X^4$ W = 1 4422495703074			
0	1 392	351	641	530	1 060	362	090	484
2	8 655	049	957	759	7 455	697	937	986
4	18 057	557	436	303	16 261	826	018	850
6	28 835	338	459	504	26 528	471	183	682
8	40 690	386	082	106	37.923	001	027	034
1	4 648	812	704	212	3 799	673	029	801
3	13.156	803	898	049	11 644	745	511	378
5	23 297	441	451	223	21.238	372	918	235
7	34 640	848	321	111	32 098	597	710	968
9	46 965	009	505	675	43 981	158	097	289

In Table 4, we present the first ten convergent energy levels of the sextic double well oscillator $V(X) = -X^2 + 0.1X^6 (\mu = 1, \lambda_1 = 1, \lambda_2 = 0, \lambda_3 = 0.1)$ and compare with that of Chaudhuri and Mondal [16] In this case, we have started from $N = 49$ and increased upto $N = 490$. Here also we find very good convergence.

Table 4. The first five (even and odd) energy levels of the Sextic-double-well-oscillator $V(X) = -X^2 + 0.1X^6 (\mu = 1, \lambda_1 = 1, \lambda_2 = 0, \lambda_3 = 0.1)$

Levels	Present (even)					Previous [16]	
0	-0 044	241	293	541	8	- 044	241
2	3 457	038	385	91		3 457	039
4	10 063	083	061	2			
6	18 549	407	539	9			
8	28 637	155	094	8			
Levels	Present (odd)					Previous [16]	
1	1 006	303	806	12		1.006	304
3	6.467	915	288	49		6.467	919
5	14 007	010	327	3			
7	23.412	470	501	7			
9	34.200	055	345	2			

In Table 5, we present the first seven convergent energy levels of the $V(X) = -2X^2 - 2X^4 + X^6$ ($\mu = 1, \lambda_1 = -2, \lambda_2 = -2, \lambda_3 = 1$) sextic-double-well-oscillator and compare results with the previous results [15, 16]. Like the previous cases, we have started from $N = 63$ and increased upto $N = 490$.

Table 5. The first three (even and odd) energy levels of the double-well-oscillator $V(X) = -2X^2 - 2X^4 + X^6$($\mu = 1, \lambda_1 = -2, \lambda_2 = -2, \lambda_3 = 1$).

Levels	Present (even)				Previous [16]		Previous [15]	
0	-1.000	000	110	6	-0.999	987	-1.0	..
2	3 629	825	916	1	3 629	880	3.629	827
4	13 350	945	225	9				
6	26 517	088	299	6				
Levels	Present (even)				Previous [16]		Previous [15]	
1	- 0.154	110	689	3	- 0.154	093		
3	8.007	560	356	4	8.007	742		
5	19 555	765	520	3				

Further, we have included only few energy levels as we do not find more results for comparison. In all cases, while computing eigenvalues, we use the appropriate value of W satisfying the limiting condition [19] $W \to \sqrt{\lambda_1}$, when $\lambda_2 \Rightarrow 0, \lambda_3 \Rightarrow 0$.

In this approach for the oscillator Hamiltonian, we find that the value of W used here is in contradiction with the Hill determinant approach of Biswas *et al* [1] where the value of W is taken as 1 *i.e.* $W = 1$. Further for the value of $W = 1$, the strength of the diagonal matrix element $< n | H | n >$ as well as the non-diagonal matrix element $< n | H | m >$ is never reduced to minimum. Perhaps this is the reason why the determinant size in the Hill determinant approach of Biswas *et al* [1] is very large. The larger the strength of the matrix element, the larger is the size of the determinant needed to yield accurate energy levels [8]. Using wave functions $|m>_{C_1}$, the strength of matrix element $< n|H|m>_{C_1}$ or $< n|H|n>_{C_1}$ (for $\mu = 1/2$ or $\lambda = 1/2$ or 1, $\lambda_2 = 1$, $\lambda_3 = 0$) in the large n limit, goes as n^2/W^2 whereas in the previous Hill determinant approach [1], it goes as n^2. For potential of the type $V(X) = X^2 + X^2 < X^m >$ where m is an even number, the present method yields the correct ground state where as variational parameter fails to yield correct ground state.

In addition to this, using the present value of W from eq. (17), we find that matrix element $< 0|H|2>_{C_1}$ turns out to be zero for the oscillator Hamiltonian *i.e.* $< 0|H|2>_{C_1} = 0$. This has been made possible due to the value of α_l. Without the value of α_l, the condition $< 0|H|2>_{C_1} = 0$ is never achieved for the oscillator Hamiltonian. It is worth mentioning that the condition $< 0 | H | 2 > = 0$ has been widely used in nuclear physics [25] to findout the most effective Hamiltonian. However for other Hamiltonians, the condition $< g|H|m> = < 1|H|2> = 0$ ($g \neq m$) should not be used to yield effective Hamiltonians. For example, consider the charmonium model potential [26] $V(r) = -\frac{1}{r} + \frac{r}{20}$. The ground state energy using α_l from eq (8) is $< 1|H|1>_{C_1} = -0.42707$ in the zeroth order approximation [27]. However, if the condition $< 1|H|2> = 0$ alone is used instead of eq.(8), then the ground state energy becomes

$<1|H|1>=-0.42645$. The exact ground state energy [26] for this Hamiltonian is $-0.428\,11$. Hence, in finding out the effective Hamiltonian for energy calculation, the role of α_l is absolutely indispensable. It is interesting to note that the present self-consistent parameter which is non-variational in nature, remains the same as variational parameter for oscillator of the type $V(X)=\lambda_1 X^2+\lambda_2 X^4+\lambda_3 X^6$. However, for oscillator of the type $V(X)=X^2+X^2<X^2>$, present self-consistent parameter is different from that of the variational parameter.

Lastly, the present method is simple and accurate. It can be applied to all oscillator potentials uniformly without any modification unlike other approximation [16, 18]. Apart from oscillator potentials, we find this approximation can also be used for non-oscillator potentials discussed elsewhere [19, 27].

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